3,4-Difluorobenzoic acid, 2-pentyl ester

Inchi: InChI=1S/C12H14F2O2/c1-3-4-8(2)16-12(15)9-5-6-10(13)11(14)7-9/h5-8H,3-4H2,1-2H3
InchiKey: PRTUHHWGVRTNKG-UHFFFAOYSA-N
Formula: C12H14F2O2
SMILES: CCCC(C)OC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 228.24

Physical Properties

Property code	Value	Unit	Source
gf	-482.67	kJ/mol	Joback Method
hf	-719.72	kJ/mol	Joback Method
hfus	25.52	kJ/mol	Joback Method
hvap	53.04	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.310		Crippen Method
mcvol	167.160	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	1352.00		NIST Webbook
tb	584.99	K	Joback Method
tc	778.46	K	Joback Method
tf	334.80	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.17	J/mol×K	584.99	Joback Method
cpg	423.81	J/mol×K	617.23	Joback Method
cpg	436.76	J/mol×K	649.48	Joback Method
cpg	449.03	J/mol×K	681.72	Joback Method
cpg	460.64	J/mol×K	713.97	Joback Method
cpg	471.58	J/mol×K	746.21	Joback Method
cpg	481.88	J/mol×K	778.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357705&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume